

ABSTRACT

[0057] A method and apparatus is used to discover elements in a compound with a fitness function by receiving a set of monoisotopic mass look-up-tables (LUTs),
5 identifying mass values in parallel by cross-referencing monoisotopic mass LUT addresses, evaluating different permutations of the identified mass values, accessing values in mass spectroscopy data sets according to the permutations of mass values and determining the combination of elements in the compound according to a correlation between the permutations of mass values and the mass values associated with the mass
10 spectroscopy data set. Performing discovery with genetic algorithms includes receiving a population of electronic chromosomes having a fitness value, selecting electronic chromosomes randomly from the population of electronic chromosomes as parent electronic chromosomes, creating child electronic chromosome through a crossover of the parent electronic chromosomes and evaluating the fitness value of the child electronic
15 chromosome to determine if the elements correspond to the compound.